UCRL- 100596 Rev. 1
PREPRINT

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THIS PAPER WAS PREPARED FOR SUBMITTAL TO
INTERNATIONAL M^2S-HTSC CONFERENCE
Stanford, CA
July 23-28, 1989

August, 1989

Lawrence Livermore National Laboratory

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We discuss our measurements of the 2D-angular correlation of positron annihilation radiation (ACAR) in La_2CuO_4, $YBa_2Cu_3O_7$ (YBCO), and NiO. The measurements for NiO are the first such 2D-ACAR measurements; the YBCO results are of a higher statistical quality than previously reported in the literature. The data are compared with complementary theoretical calculations and with each other. We discuss the implication of our analysis for ACAR studies of similar and related systems.

1. INTRODUCTION

In recent months, the positron-annihilation technique has assumed a useful role in the elucidation of the physics of the new high-critical temperature superconductors. ACAR techniques have been used to probe the electronic momentum densities. Although similar results have been obtained by many workers, the interpretations have been controversial.[1] On the basis of high statistical quality ACAR measurements of La_2CuO_4, $YBa_2Cu_3O_{7-\delta}$, and NiO, our positron lifetime studies,[2] preliminary calculations of the positron wave function, and theoretical calculations based upon a LCAO-MO model within the independent-particle model,[3] we offer a consistent and preliminary interpretation of the ACAR results for high-T_c and related systems. Our findings for La_2CuO_4 and NiO have been published elsewhere[3,4]; the YBCO results will be published shortly.[5] Some of the new YBCO results will be presented here.

2. EXPERIMENT

Two-dimensional ACAR measurements were performed upon the La_2CuO_4 and YBCO samples at RT and NiO at 13K. The sample-to-detector distance was 9.6m [11m] for La_2CuO_4 and NiO [YBCO]; the combined angular resolution of the detectors was 0.50 mrad [0.80 mrad]. 1 mrad corresponds to an electron -positron momentum of $10^{-3}mc$, where m is the electron rest mass. The La_2CuO_4 and NiO [YBCO] measurements consisted of 16 to 50 million counts, ~10^4 counts peak channel, in a 256x256 [128x128] square matrix with a bin width of (0.208 mrad)^2 [(0.38 mrad)^2]. Momentum integration directions were along high-symmetry sample crystalline axes (<100> and <110>).

The La_2CuO_4 and NiO samples have been described elsewhere.[3,4] The YBCO measurements were made upon an oriented mosaic of four crystals (~1x1x.06) mm^3 grown by Z. Z. Wang of Princeton

* Work performed under the auspices of the U.S. Dept. of Energy by the Lawrence Livermore Natl. Laboratory under contract No.W-7405-ENG-48.

University. Meissner-effect measurements of the crystals before and after the ACAR experiments showed T_c between 90 and 93K, with $\Delta T \approx 0.5K$. Positron annihilation lifetime measurements made upon these samples showed no evidence of defect trapping.[3,4]

3. RESULTS AND DISCUSSION

The ACAR electron-positron momentum distributions we obtained were qualitatively similar: highly isotropic with no statistically significant "Fermi breaks" due to partially-filled band contributions. The highly isotropic nature of the distributions suggests a significant (80 to 90%) "core state" contribution.[3-5] We have successfully modeled the small anisotropic valence-electron contribution to these distributions using an LCAO-MO formalism in conjunction with the IPM. The positronic wave function, in a Bloch state with zero momentum, is modeled using a variational procedure which takes properly into account the fairly localized electronic character of the material and also the relative affinity of the positron to the different chemical species.[3]

The statistically significant anisotropic components of the experimental distributions and their theoretical counterparts were in qualitative agreement. This illustrates the utility of our method for probing selected details of the interatomic bonding in these systems. See Fig. 1 for an example and Refs.3-5 for extended discussion. The anisotropies in the experimental spectra reflect, in the main, the spatial distribution of the electron and positron charge densities rather than the fine details of the electronic band-structure.

4. CONCLUSION

Our ACAR studies show that: 1) positrons are significantly sensitive to non-conduction electrons and details of the Cu-O bonding in high-T_c materials and related systems and 2) the contributions of the probing positron to the ACAR distributions are important and non-trivial. Such "positron wavefunction" effects must be taken into account in future ACAR studies. Higher-statistics, higher-resolution and higher-accuracy ACAR measurements are probably required to conclusively establish the existence of a Fermi surface in YBCO.

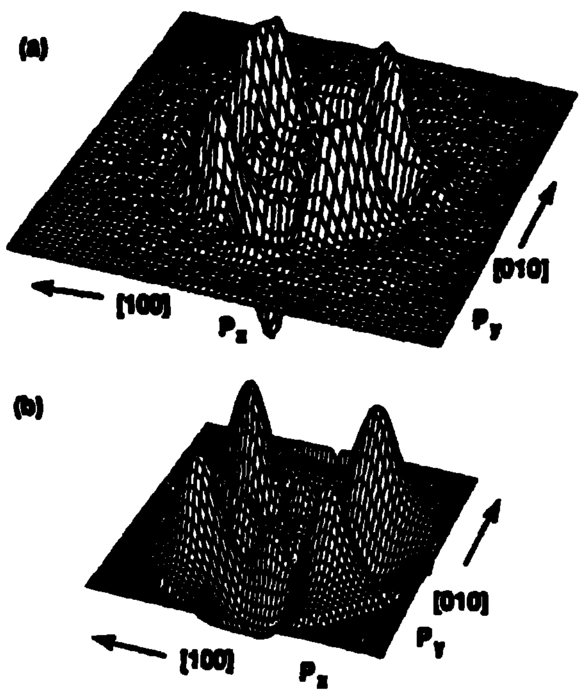

FIGURE 1

Experimental a) and theoretical b) residual anisotropy surfaces for $YBa_2Cu_3O_7$. The momentum integration direction is the c-axis. The values of p_x and p_y range between $\pm$ 21.8 mrad (a) and $\pm$ 15 mrad (b).

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